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A one-Fermion-one-Boson model for a magnetic elastic system

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Abstract. A highly simplified model of a spin system interacting with a vibration mode is presented. It is shown to lead to the Hamiltonian $\omega b^+ b + Jc^+ c + \alpha(b + b^+)(c + c^+)$ where b, b^+ and c, c^+ are Boson and Fermion operators, respectively. Some general exact properties (including energy bounds) as well as various approximations of the associated eigenvalues and eigenstates are derived.

1. The Problem

In elastic magnetic crystals the Heisenberg model must be modified so as to include a spatial dependence of the Heisenberg coupling constant (see e.g. [1], [2]). This dependence obviously induces a coupling between phonons and the spin system of the crystal. This coupling has been extensively studied by Imboden [3] in the case of small Curie temperature (compared to the Debye temperature; i.e. high phonon frequencies and weak magnetic coupling) and weak spatial dependence. As these assumptions are sometimes too restrictive, however, it is the aim of this note to give an account of what may occur when they are not fulfilled. The problem of working out the detailed structure of such a crystal is hopelessly complicated, so consideration is limited to a grossly simplified but perhaps nonetheless suggestive model. Actually, even this model turns out not to be exactly solvable.

We shall consider a triatomic magnetic molecule with both ends fixed. The three spins are assumed to be $\frac{1}{2}$. The corresponding general Hamiltonian is

$$H = (\omega/2)(-(d^2/dx^2) + x^2 - 1) \otimes \mathbb{1} - \mathbb{1} \otimes J(\mathbf{s}_1 \cdot \mathbf{s}_2 + \mathbf{s}_2 \cdot \mathbf{s}_3) + I(x) \otimes (\mathbf{s}_1 \cdot \mathbf{s}_2 - \mathbf{s}_2 \cdot \mathbf{s}_3), \quad (1)$$

where $\mathbf{s}_i$ denote the spin operators. We now define creation and annihilation operators for Bosons by

$$b^+ = (-(d/dx) + x)/\sqrt{2}, \qquad b = ((d/dx) + x)/\sqrt{2}.$$

For the sake of simplicity we further take $I(x)$ to be linear. $\omega > 0$, J, α being real parameters, the model Hamiltonian is thus given by

$$H = \omega b^+ b \otimes \mathbb{1} - \mathbb{1} \otimes J(\mathbf{s}_1 \cdot \mathbf{s}_2 + \mathbf{s}_2 \cdot \mathbf{s}_3) + \alpha(b + b^+) \otimes (\mathbf{s}_1 \cdot \mathbf{s}_2 - \mathbf{s}_2 \cdot \mathbf{s}_3). \quad (2)$$

2. Symmetries of the Hamiltonian

We now proceed to reduce the Hamiltonian (2) to a more tractable form and to examine its symmetries. First, it is obvious that

$$\left[H, \sum_{i=1}^{3} s_i^z\right] = \left[H, \left(\sum_{i=1}^{3} \mathbf{s}_i\right)^2\right] = 0.$$

This makes it possible to consider the Hamiltonian only on subspaces invariant under $\sum_{i=1}^3 s_i^z$ and $(\sum_{i=1}^3 \mathbf{s}_i)^2$. There are only two such subspaces which are non-trivial, i.e. have dimension greater than one. These are clearly isomorphic, however, so we shall from now on restrict ourselves to one single two-dimensional subspace of the whole 8-dimensional spin space, namely the one spanned by the vectors

$$|\varphi\rangle = (|\uparrow\uparrow\downarrow\rangle - 2|\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle)/\sqrt{6},$$
$$|\chi\rangle = (|\uparrow\uparrow\downarrow\rangle - |\downarrow\uparrow\uparrow\rangle)/\sqrt{2},$$

with selfexplanatory notation. We now define the following vectors and operators:

$$|n\rangle = (n!)^{-1/2}(b^+)^n|0\rangle, \quad \text{where } b|0\rangle = 0;$$
$$|n, \varphi\rangle = |n\rangle \otimes |\varphi\rangle, \qquad |n, \chi\rangle = |n\rangle \otimes |\chi\rangle;$$
$$c^+|\varphi\rangle = 0, \qquad c^+|\chi\rangle = |\varphi\rangle;$$
$$c|\varphi\rangle = |\chi\rangle, \qquad c|\chi\rangle = 0.$$

Evidently, c^+ and c have all the properties of creation and annihilation operators for Fermions. The spin system of the whole molecule has therefore been effectively reduced to one single two-level system. Accordingly, the Hamiltonian (2) now takes the form

$$H = \omega b^+ b + J c^+ c + \alpha(b + b^+)(c + c^+), \quad (3)$$

where we have dropped the tensor products and written b for $b \otimes \mathbb{1}$ etc. Henceforth we shall consider (3) as our basic Hamiltonian. Of the vast literature on this and related Hamiltonians we only mention [4], [5], and [6] as some landmarks for the discussion of the eigenvalue problem associated with (3).

There is yet one symmetry of some importance to be considered. On physical grounds it is reasonable to expect that the model is symmetric with respect to the centre of the molecule, which has all the while been taken to be the origin. This corresponds to the transformation $P:(x, \mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3) \mapsto (-x, \mathbf{s}_3, \mathbf{s}_2, \mathbf{s}_1)$, and indeed one immediately finds that this parity operator P commutes with (2). Alternatively, the relations

$$P|n, \varphi\rangle = (-1)^n|n, \varphi\rangle, \quad P|n, \chi\rangle = (-1)^{n+1}|n, \chi\rangle$$

imply

$$P = -(-1)^{b^+b+c^+c},$$

which also manifestly commutes with (3). The fact that $(-1)^{b^+b+c^+c}$ is a constant of motion for (3) seems to have been overlooked in most of the literature apart from [7] and [8]. Whether there exist any additional symmetries (i.e. parameter-independent constants of motion) will later be shown to be a question of some relevance.

3. Exactly solvable related models

We first wish to discuss two important exactly solvable special cases of (3): $\alpha = 0$ and $J = 0$, respectively. In the case $\alpha = 0$, it is clear that $|n, \varphi\rangle$ and $|n, \chi\rangle$ are eigenvectors to the energies $\omega n + J$ and ωn, respectively. In the case $J = 0$, define

$$\begin{aligned} |n \pm\rangle &= \exp(-\alpha^2/2\omega^2)(n!)^{-1/2}(b^+ \pm \alpha/\omega)^n \exp(\mp(\alpha/\omega)b^+)|0\rangle, \\ |\vartheta \pm\rangle &= (|\varphi\rangle \pm |\chi\rangle)/\sqrt{2}, \\ |n\pm, \vartheta\pm\rangle &= |n\pm\rangle \otimes |\vartheta\pm\rangle. \end{aligned} \tag{4}$$

One easily verifies that $|n\pm, \vartheta\pm\rangle$ are both eigenvectors to the same degenerate eigenvalue $\omega n - \alpha^2/\omega$. We therefore note that, whenever $|J| = n\omega$ and $\alpha = 0$, degeneracies appear from the nth excited level upwards. In the case of $J = 0$ this degeneracy persists even when $\alpha \neq 0$.

Second, we consider (3) for the case $J \cong \omega$. It can then be shown that, at least for small $|\alpha|$, the main contribution to the energy is given by the rotating wave approximation

$$\tilde{H} = \omega b^+b + Jc^+c + \alpha(b^+c + bc^+),$$

which is exactly solvable. The energies are

$$\omega(n-1) + \tfrac{1}{2}(J+\omega) \pm [\tfrac{1}{4}(J-\omega)^2 + \alpha^2 n]^{1/2},$$

and the corresponding eigenstates are linear combinations of $|n-1, \varphi\rangle$ and $|n, \chi\rangle$, therefore being also eigenvectors of P with eigenvalue (parity) $(-1)^{n+1}$. The ground state turns out to be $|0, \chi\rangle$ so long as $\alpha^2 \leqslant \omega|J|$. Otherwise it becomes a linear combination of $|n, \varphi\rangle$ and $|n+1, \chi\rangle$ where n takes successively all values 0, 1, ... with increasing $|\alpha|$. This means in particular that the ground state of H has alternating parity with increasing $|\alpha|$. In contradistinction to this, it will be shown in section 4 that the ground state of H has α-independent parity. Further, if H has no symmetries other than the parity operator P, then a standard argument due to Wigner and von Neumann (see e.g. [9], p. 262) makes it plausible that the ground state of H is always nondegenerate apart from exceptional isolated values of *both* α/ω and J/ω. This is due to the fact that two ground states of H would necessarily both have the same parity and thus the same symmetry. This is again in contrast to the behaviour of $\tilde{H}$ where, for each value of α/ω there exist infinitely many values of J/ω for which the ground state is twofold degenerate.

4. Exact properties of the eigenstates

We first wish to determine the asymmetry of the spatial and spin configurations of any of the eigenstates $|\psi\rangle$ of (3), i.e. to determine $\langle\psi|b + b^+|\psi\rangle$ and $\langle\psi|c + c^+|\psi\rangle$ (since $c + c^+$ is proportional to $\mathbf{s}_1 \cdot \mathbf{s}_2 - \mathbf{s}_2 \cdot \mathbf{s}_3$ the quantity $\langle\psi|c + c^+|\psi\rangle$ does indeed give a measure of the asymmetry of the spin system). It is easily seen that both are identically zero: For the eigenstates of H can always be chosen to be eigenvectors of P, so that for example

$$\langle\psi|b + b^+|\psi\rangle = \langle\psi|P(b + b^+)P|\psi\rangle = -\langle\psi|b + b^+|\psi\rangle.$$

We now show that the eigenstates of the Hamiltonian (3) are in a sense asymtotically coherent states: Let

$$|\psi^{(+)}\rangle = \sum_{n=0}^{\infty} (a_{2n}^{(+)}|2n, \varphi\rangle + a_{2n+1}^{(+)}|2n + 1, \chi\rangle)$$

$$|\psi^{(-)}\rangle = \sum_{n=0}^{\infty} (a_{2n}^{(-)}|2n, \chi\rangle + a_{2n+1}^{(-)}|2n + 1, \varphi\rangle)$$

be eigenstates of the Hamiltonian (3) with parity + 1 and − 1, respectively. Then the coefficients $a_n^{(\pm)}$ satisfy

$$a_n^{(\pm)} = (-\alpha/\omega)^n (n!)^{-1/2} g_n^{(\pm)} \quad \text{for } n \to \infty,$$

where $g_n^{(\pm)} > 0$ and $\max(g_n^{(\pm)}, 1/g_n^{(\pm)}) = O(n^\lambda)$ for some $\lambda > 0$ (dependent on the corresponding energy eigenvalue).

Proof: The eigenvalue equation for $|\psi^{(\pm)}\rangle$ and the corresponding eigenvalue $E^{(\pm)}$ reduces to the following difference equation for the $a_n^{(\pm)}$:

$$[\omega n + \tfrac{1}{2}J(1 \pm (-1)^n)]a_n^{(\pm)} + \alpha(\sqrt{n+1}\, a_{n+1}^{(\pm)} + \sqrt{n}\, a_{n-1}^{(\pm)}) = E^{(\pm)} a_n^{(\pm)}.$$

Define now

$$r_n^{(\pm)} = -(\sqrt{n+1}\,\omega/\alpha) a_{n+1}^{(\pm)}/a_n^{(\pm)},$$

where $r_n^{(\pm)}$ is set equal to $-\infty$ whenever $a_n^{(\pm)} = 0$. The recursion formula for $r_n^{(\pm)}$ is then

$$r_n^{(\pm)} = (\omega/\alpha^2)[\omega n + \tfrac{1}{2}J(1 \pm (-1)^n) - E^{(\pm)} - (\omega n / r_{n-1}^{(\pm)})].$$

By studying the rate of growth of $r_n^{(\pm)}$ and comparing with $a_n^{(\pm)}$ one obtains that

$$\sum_{n=0}^{\infty} |a_n^{(\pm)}|^2 < \infty \quad \text{if and only if } \lim_{n\to\infty} r_n^{(\pm)} = 1,$$

wherefrom the stated asymptotic property for $a_n^{(\pm)}$ is obvious. Q.E.D.

Finally we prove the result announced in section 3 that the ground state of H has α-independent parity: The restriction of the Hamiltonian (3) to a subspace of fixed parity ± 1 is given by

$$H^{(\pm)} = \omega \tilde{b}^+ \tilde{b} \pm J(-1)\tilde{b} + \tilde{b} + \alpha(\tilde{b} + \tilde{b}^+) + J/2,$$

where $\tilde{b} = b(c + c^+)$ and $\tilde{b}^+ = b^+(c + c^+)$ satisfy the commutation relations for Bosons. Using the Dyson series with $\omega \tilde{b}^+ \tilde{b} + \alpha(\tilde{b} + \tilde{b}^+)$ as the unperturbed Hamil-

tonian, and taking the trace by means of coherent states, a straightforward but tedious calculation yields

$$tr\, e^{-\beta H^{(\pm)}} = \sum_{n=0}^{\infty} A_n(\beta)(\pm J)^n e^{-\beta J/2},$$

where $A_n(\beta) > 0$. Assuming $J > 0$, the equation

$$E^{(\pm)} = -\lim_{\beta\to\infty}(1/\beta)\ln tr\, e^{-\beta H^{(\pm)}}$$

for the ground state energy $E^{(\pm)}$ of $H^{(\pm)}$ then implies $E^{(+)} \leqslant E^{(-)}$, which in turn shows that the parity of the ground state is 1. Similarly, for $J < 0$ the ground state has parity -1. This result gives some additional insight into the degeneracy of the ground state at $J = 0$: It obviously is due to the coincidence of two states of opposite parity.

5. Approximations

In some particular situations there are methods of finding the eigenstates and eigenvalues of (3) to a fairly good approximation: The cases $|\alpha| \ll \omega, |J|$ and $|J| \ll \omega$ will be treated by ordinary perturbation theory, whereas consideration of the strong coupling region $\omega \ll \max(|J|,|\alpha|)$ will cover the cases $\alpha^2 \ll \omega|J|$ and $\omega|J| \ll \alpha^2$ (see Figure 1).

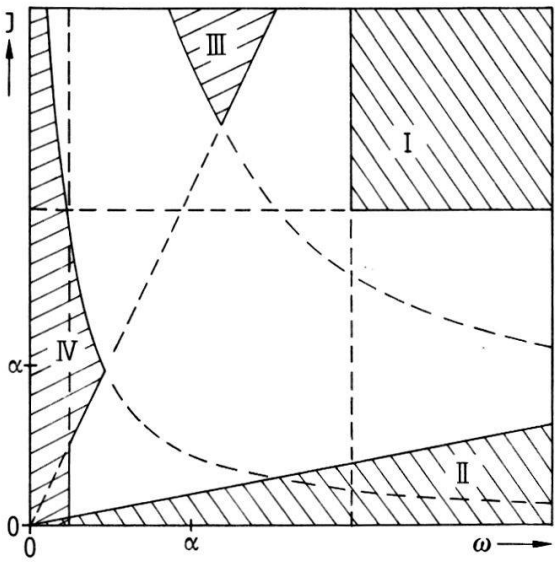

Figure 1
Schematic representation (for variable ω, J and fixed α) of the domains of validity (shaded areas) of the various approximations.

I: $|\alpha| \ll \omega, |J|$ III: $\omega \ll \max(|J|, |\alpha|)$; $\alpha^2 \ll \omega|J|$
II: $|J| \ll \omega$ IV: $\omega \ll \max(|J|, |\alpha|)$; $\omega|J| \ll \alpha^2$

5.1 Perturbation theory

Taking H with $\alpha = 0$ and $J = 0$, respectively, as unperturbed operator, perturbation theory to the lowest significant order requires the distinction of the following three cases (cf. Figure 1):

$|\alpha| \ll \omega, |J|; |J| \neq \omega$. Usual perturbation theory works even if $|J| = n\omega$ with $n > 1$ because in this case the splitting of the degenerate eigenvalues occurs only in higher orders of α. The eigenstates are given by

$$|n, \chi\rangle + \alpha\left(\frac{\sqrt{n}}{\omega - J}|n-1, \varphi\rangle - \frac{\sqrt{n+1}}{\omega + J}|n+1, \varphi\rangle\right) + O(\alpha^2), \tag{5}$$

$$|n, \varphi\rangle - \alpha\left(\frac{\sqrt{n+1}}{\omega - J}|n+1, \chi\rangle - \frac{\sqrt{n}}{\omega + J}|n-1, \chi\rangle\right) + O(\alpha^2), \tag{6}$$

and the corresponding eigenvalues by

$$\omega n - \alpha^2\left(\frac{n+1}{\omega + J} - \frac{n}{\omega - J}\right) + O(\alpha^4),$$

$$\omega n + J + \alpha^2\left(\frac{n}{\omega + J} - \frac{n+1}{\omega - J}\right) + O(\alpha^4).$$

$|\alpha| \ll \omega, |J|; |J| = \omega$. Here it must be remembered that all the excited states of the unperturbed Hamiltonian are degenerate. For $J > 0$, i.e. $J = \omega$ we obtain

$$(|n, \chi\rangle \pm |n-1, \varphi\rangle)/\sqrt{2} + O(\alpha), \tag{7}$$
$$\omega n \pm \alpha\sqrt{n} + O(\alpha^2)$$

for the eigenstates and eigenvalues, respectively. It must be emphasized that these formulae do not concern the ground state which is nondegenerate. It further is to be noted that the energy of the excited states is now subjected to a linear contribution in α instead of a quadratic one as in the case of $|J| \neq \omega$. This effect is of resonant type.

$|J| \ll \omega$. Here the eigenvalues of the unperturbed problem are twofold degenerate. This gives

$$(|n+, \vartheta+\rangle \pm |n-, \vartheta-\rangle)/\sqrt{2} + O(J), \tag{8}$$
$$\omega n - \alpha^2/\omega + \tfrac{1}{2}(J \pm J) + O(J^2)$$

for the eigenvectors and eigenvalues, respectively. Thus the energies corresponding to the minus sign and all eigenvalues are affected by the perturbation only in second order.

The fact that the above approximate eigenstates (5), ..., (8) all are eigenvectors of the parity operator P, is in good accordance with the corresponding property of the exact eigenstates. In particular, it follows that $\langle b + b^+\rangle = \langle c + c^+\rangle = 0$ if the expectation value $\langle \cdots \rangle$ is taken with respect to any of the states (5), ..., (8) (cf. section 4). Furthermore, it is of interest to calculate the expectation value of $(b + b^+) \times$

$\times (c + c^+)$ as it is a measure for the correlation between the asymmetry of the spin system and the displacement: For the states (5) and (6) one finds

$$\langle (b + b^+)(c + c^+) \rangle = 2\alpha((2n + 1)J + \omega)/(J^2 - \omega^2) + O(\alpha^2),$$
$$\langle (b + b^+)(c + c^+) \rangle = 2\alpha((2n + 1)J - \omega)/(J^2 - \omega^2) + O(\alpha^2),$$

respectively, whereas the states (7) yield

$$\langle (b + b^+)(c + c^+) \rangle = \pm 2\sqrt{n} + O(\alpha).$$

We thus have the rather remarkable result that the correlation $\langle (b + b^+)(c + c^+) \rangle$ tends to 0 as $\alpha \to 0$ only in the nonresonant case $|J| \neq \omega$. Finally, for the situation $|J| \ll \omega$, i.e. for the states (8) one obtains

$$\langle (b + b^+)(c + c^+) \rangle = -2\alpha/\omega + O(J),$$

which is (at least for reasonably small n) in accordance with the above result for the states (5) and (6) when $|\alpha| \ll |J| \ll \omega$. Here independence of n is the most remarkable feature, as well as the fact that the correlation is always negative (in contrast to the result for the states (5), (6), and (7)).

5.2 *Strong coupling*

We will now show that under certain restrictions the motion of the system can be described either as a motion in a double-well potential or in a harmonic potential centred at the origin, depending on whether $\alpha^2 \gg \omega|J|$ or $\alpha^2 \ll \omega|J|$. As we shall be concerned with small ω, it is convenient to rescale the Schrödinger equation as follows: Let

$$|\psi\rangle = |\psi_1\rangle \otimes |\vartheta+\rangle + |\psi_2\rangle \otimes |\vartheta-\rangle$$

be an eigenvector to the energy E. The equations for ψ_1 and ψ_2 then read

$$\begin{aligned} -\tfrac{1}{2}\omega\psi_1''(x) + \tfrac{1}{2}\omega x^2\psi_1(x) + \sqrt{2}\,\alpha x\psi_1(x) + \tfrac{1}{2}J\psi_2(x) &= (E + \tfrac{1}{2}(\omega - J))\psi_1(x), \\ -\tfrac{1}{2}\omega\psi_2''(x) + \tfrac{1}{2}\omega x^2\psi_2(x) - \sqrt{2}\,\alpha x\psi_2(x) + \tfrac{1}{2}J\psi_1(x) &= (E + \tfrac{1}{2}(\omega - J))\psi_2(x). \end{aligned} \tag{9}$$

Introducing the notation

$$y = (\omega/\sqrt{8}\,\alpha)x, \qquad \tilde{\psi}_j(y) = \psi_j(x),$$
$$\kappa = 4\alpha^2/\omega, \qquad \tilde{E} = E + \tfrac{1}{2}(\omega - J + \tfrac{1}{2}\kappa),$$

one obtains

$$\begin{aligned} (-\omega^2/4\kappa)\tilde{\psi}_1''(y) + \kappa(y + \tfrac{1}{2})^2\tilde{\psi}_1(y) + \tfrac{1}{2}J\tilde{\psi}_2(y) &= \tilde{E}\tilde{\psi}_1(y), \\ (-\omega^2/4\kappa)\tilde{\psi}_2''(y) + \kappa(y - \tfrac{1}{2})^2\tilde{\psi}_2(y) + \tfrac{1}{2}J\tilde{\psi}_1(y) &= \tilde{E}\tilde{\psi}_2(y). \end{aligned} \tag{10}$$

We now consider strong coupling, that is ω small and κ fixed. This limit is not well-defined since the parameter taken to be small occurs in the highest derivative. It can be shown that for $\omega \to 0$ the Hamiltonian corresponding to (10) converges towards the Hamiltonian for $\omega = 0$ in the strong resolvent sense only (see [10]). It is therefore to be expected that only results of a qualitative, at best of an asymptotic character will hold.

We first note once and for all that it is sufficient to find either $\tilde{\psi}_1$ or $\tilde{\psi}_2$ since for example

$$\tilde{\psi}_2(y) = \tilde{\psi}_1(-y) \tag{11}$$

satisfies equations (10). This reflects parity conservation.

The spectrum of the system (10) for $\omega = 0$ is easily found to be given by

$$V^{(\pm)}(\eta) = \kappa(\eta^2 + \tfrac{1}{4}) \pm (\tfrac{1}{4}J^2 + \kappa^2\eta^2)^{1/2}, \quad -\infty < \eta < \infty.$$

The generalized eigenfunctions belonging to the element ε of the spectrum of the system (10) for $\omega = 0$ are of the form

$$\tilde{\psi}_1(y) = \tilde{\psi}_2(-y) = \sum_{\pm} \sum_{i} d_i^{(\pm)} \delta(y - y_i^{(\pm)})$$

where the $d_i^{(\pm)}$ are arbitrary coefficients and the $y_i^{(\pm)}$ are defined by the equation

$$V^{(\pm)}(y_i^{(\pm)}) = \varepsilon. \tag{12}$$

We will assume that the difference between the two energy curves $V^{(+)}$ and $V^{(-)}$ is everywhere large compared to ω. This is certainly so if $|J| \gg \omega$; moreover, it is also true if $\kappa \gg \omega$ and $\eta \neq 0$. It will later be made plausible, however, that in this latter case the wave functions $\tilde{\psi}_1$ and $\tilde{\psi}_2$ vanish exponentially with κ at $y = 0$. Therefore the following considerations will hold whenever $\max(|J|, |\alpha|) \gg \omega$. Under these hypotheses it appears justified to take an eigenstate of the full Hamiltonian to be a superposition of states belonging to a fixed energy curve, i.e. either to $V^{(+)}$ or to $V^{(-)}$. We will confine our attention to $V^{(-)}$ as it obviously is the important one for low excited states. In higher excited states it is not clear whether the transitions between the two energy curves can be neglected. We further admit that the kinetic energy will not cause transitions between states localized wide apart. Altogether this leads to the ansatz

$$\tilde{\psi}_1(y) = \tilde{\psi}_2(-y) = \sum_i f_i(y),$$

where each f_i is some function sharply peaked around $y_i^{(-)}$ and the $y_i^{(-)}$ are as in (12), ε being considered as variation parameter. We then wish to find a normalized $\tilde{\psi} = (\tilde{\psi}_1, \tilde{\psi}_2)$ such that the expectation value of the Hamiltonian corresponding to the left-hand side of (10) remains stationary. Within the above approximation, this expectation value is proportional to

$$\langle\tilde{\psi}_1| - \frac{\omega^2}{4\kappa}\frac{d^2}{dy^2} + V^{(-)}(y)|\tilde{\psi}_1\rangle + \langle\tilde{\psi}_2| - \frac{\omega^2}{4\kappa}\frac{d^2}{dy^2} + V^{(-)}(y)|\tilde{\psi}_2\rangle$$

(actually we could have written ε for $V^{(-)}(y)$ in this approximation; however, by using $V^{(-)}(y)$ instead, we avoid dependence of the operator on the variation parameter). If this is to be stationary then the following equations must hold:

$$(-\omega^2/4\kappa)\tilde{\psi}_j''(y) + V^{(-)}(y)\tilde{\psi}_j(y) = \tilde{E}^{ad}\tilde{\psi}_j(y), \quad j = 1, 2. \tag{13}$$

This approximation is closely related to the Born–Oppenheimer (or adiabatic) approximation. Indeed (13) could also have been derived from the following physical considerations: For ω small, the coupling between the spin system and the displacement of the central ion becomes so important that the spin system adjusts itself to the instantaneous spatial configuration. This is in perfect analogy with the adiabatic

adjustment of the electronic states to the nuclear configuration presupposed by the Born–Oppenheimer approximation. The energy of the "adjusted" spin configuration as a function of the displacement is then taken as a multiplication operator in the Hamiltonian of the phonon system alone, where it plays the part of an additional potential, again as in the Born–Oppenheimer method.

Solving the eigenvalue equations (13) analytically is not possible. Instead we will discuss qualitatively the following two situations (cf. Figure 1; note that we still have the requirement $\omega \ll \max(|J|, |\alpha|)$):

$\underline{\kappa \ll |J|}$. The potential $V^{(-)}$ takes the form

$$V^{(-)}(y) = \kappa(1 - \kappa/|J|)y^2 + \kappa/4 - |J|/2 + O(y^3)$$

for y near zero. This gives an harmonic potential which can obviously be solved exactly.

$\underline{|J| \ll \kappa}$. Here the potential $V^{(-)}$ can be approximated by

$$V^{(-)}(y) = \kappa(y^2 + \tfrac{1}{4}) - \kappa|y| + O(1/y)$$

Approximate solutions of the corresponding symmetrical double-well potential problem may be obtained as the sum and difference of oscillator eigenfunctions translated by $\pm\frac{1}{2}$, i.e. of coherent states. It is to be noted that the symmetry of the double-well potential is largely accidental and certainly not due to parity conservation. The distribution of the eigenvalues is also remarkable: They are each quasi-twofold degenerate corresponding to even and odd solutions. The level splitting is given by the tunnelling frequency which decreases exponentially with κ, whereas the location of these doublets is approximately where the single eigenvalues of the simple displaced harmonic oscillator would be. In particular, it follows that the lowest eigenvalues are of the order ω for the system (10), and of the order $-\frac{1}{4}\kappa$ for the system (9).

We now give a completely different account of the behaviour of the system for $|J|, \omega \ll \kappa$. By solving the second equation of (10) for $\tilde{\psi}_2$ and inserting in the first equation we obtain

$$-(\omega^2/4\kappa)\tilde{\psi}_1''(y) + \kappa(y + \tfrac{1}{2})^2\tilde{\psi}_1(y)$$

$$+ \tfrac{1}{2}(J^2/\sqrt{\omega\kappa}) \int_{-\infty}^{\infty} G_\nu(\kappa/\omega; y, \eta)\tilde{\psi}_1(\eta)d\eta = \tilde{E}\tilde{\psi}_1(y), \tag{14}$$

where

$$\nu = \tilde{E}/\omega - \tfrac{1}{2},$$

$$G_\nu(\kappa/\omega; y, \eta) = \begin{cases} \dfrac{\Gamma(-\nu)}{2\sqrt{2\pi}} D_\nu\left(2\sqrt{\dfrac{\kappa}{\omega}}(y - \tfrac{1}{2})\right) D_\nu\left(-2\sqrt{\dfrac{\kappa}{\omega}}(\eta - \tfrac{1}{2})\right) & \text{if } \eta \leqslant y \\ \dfrac{\Gamma(-\nu)}{2\sqrt{2\pi}} D_\nu\left(-2\sqrt{\dfrac{\kappa}{\omega}}(y - \tfrac{1}{2})\right) D_\nu\left(2\sqrt{\dfrac{\kappa}{\omega}}(\eta - \tfrac{1}{2})\right) & \text{if } \eta > y \end{cases},$$

and D_ν are the parabolic cylinder functions as defined in [11]. Taking $\tilde{\psi}_1$ to be an oscillator eigenfunction displaced by $-\frac{1}{2}$, the condition that (14) be approximately satisfied implies that

$$\frac{1}{2}\frac{J^2}{\sqrt{\omega\kappa}}\int_{-\infty}^{\infty} G_\nu(\kappa/\omega; y, \eta)\ \tilde{\psi}_1(\eta)d\eta$$

be small. Using the asymptotic formulae for the parabolic cylinder functions with large argument and moderate index (see e.g. [11], p. 348) and approximations of the type

$$\int_{-\infty}^{y} e^{-a\eta^2} f(\eta)d\eta \cong \tfrac{1}{2}(\pi/a)^{1/2} e^{-ay^2} f(y)$$

for $y < 0$ and a large, one easily finds that the above integral is indeed small. According to equation (11) we get thus $(\tilde{\psi}_1(y), \tilde{\psi}_1(-y))$ as an approximation to the solution of (10). On the other hand, $\tilde{\psi}_2$ may also be obtained by considering the integro-differential equation analogous to (14) for $\tilde{\psi}_2$, which yields $\tilde{\psi}_2(y) \cong \pm\,\tilde{\psi}_1(-y)$; by choosing the minus sign we then find $(\tilde{\psi}_1(y), -\tilde{\psi}_1(-y))$ as a quasi-degenerate second solution of (10). All this is therefore in rather good agreement with the double-well description given above.

It has not been possible to carry such calculations over to the case $|J| \gg \kappa$, although this would certainly be desirable in order to confirm that the particle then indeed is located at the origin. The reason for this difficulty stems from the fact that, for $|J| \gg \kappa$, the nonlocal character of the problem (due to the integral term in equation (14)) becomes dominant.

6. Ground state energy bounds

Putting $\sigma = \omega^2 + J^2$ and $\rho = [(\omega^2 - J^2)^2 + 16\alpha^2\omega|J|]^{1/2}$,
the following inequalities hold for the ground state energy E of the Hamiltonian (3):

$$E \geqslant E_{\mathrm{I}} = -\frac{\alpha^2}{\omega} + \tfrac{1}{2}(J - |J|)$$

$$E \geqslant E_{\mathrm{II}} = \left\{ \begin{array}{ll} -\dfrac{\alpha^2}{\omega} - \dfrac{\omega J^2}{16\alpha^2} + \tfrac{1}{2}(J - \omega) & \text{if } 4\alpha^2 \geqslant \omega|J| \\ \tfrac{1}{2}(J - |J| - \omega) & \text{else} \end{array} \right\}$$

$$\left.\begin{array}{l} E \geqslant E_{\mathrm{III}} = \dfrac{1}{2\sqrt{2}}(\sqrt{\sigma + \rho} + \sqrt{\sigma - \rho}) + \tfrac{1}{2}(J - \omega) - |J| \\ \geqslant E_{\mathrm{IV}} = \tfrac{1}{2}\omega\left[\left(1 - \dfrac{4\alpha^2}{\omega|J|}\right)^{1/2} - 1\right] + \tfrac{1}{2}(J - |J|) \\ \geqslant E_{\mathrm{II}} \end{array}\right\} \text{for } 4\alpha^2 \leqslant \omega|J|$$

$$E \leqslant E_{\mathrm{V}} = \min_{\gamma} (\omega\gamma^2 + 2|\alpha|\gamma - \tfrac{1}{2}|J|e^{-2\gamma^2} + \tfrac{1}{2}J)$$

$$E \leqslant E_{\mathrm{VI}} = \left\{ \begin{array}{ll} -\dfrac{\alpha^2}{\omega} - \dfrac{\omega J^2}{16\alpha^2} + \tfrac{1}{2}J & \text{if } 4\alpha^2 \geqslant \omega|J| \\ \tfrac{1}{2}(J - |J|) & \text{else} \end{array} \right\}$$

$$\leqslant E_{\mathrm{VII}} = -\frac{\alpha^2}{\omega} + \tfrac{1}{2}(J + |J|).$$

Proof: The bounds E_{I} and E_{VII} are immediate consequences of the operator inequality $0 \leqslant c^+c \leqslant \mathbb{1}$ and of $-\alpha^2/\omega$ being the ground state energy of (3) with $J = 0$.

The lower bounds E_{II} and E_{IV} are obtained from a variant of the Brattsev-Epstein inequality, stating that for molecular Hamiltonians the exact adiabatic ground state energy is a lower bound for the exact ground state energy. Here we follow the lines of the proof given in [12] in order to show that the ground state energy $\tilde{E}^{\mathrm{ad}}$ of (13) is a lower bound for the ground state energy $\tilde{E}$ of (10): Define

$$T = -\frac{\omega^2}{4\kappa}\frac{d^2}{dy^2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$M = \begin{pmatrix} \kappa(y + \tfrac{1}{2})^2 & J \\ J & \kappa(y - \tfrac{1}{2})^2 \end{pmatrix}, \quad M^{\mathrm{ad}} = V^{(-)}(y)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then the Hamiltonians associated with the eigenvalue problems (10) and (13) are given by $T + M$ and $T + M^{\mathrm{ad}}$, respectively. Furthermore, the variational principle clearly implies the operator inequality $M \geqslant M^{\mathrm{ad}}$. For the exact (normalized) ground state $\tilde{\psi} = (\tilde{\psi}_1, \tilde{\psi}_2)$ of (10) this leads to

$$\tilde{E} = \langle \tilde{\psi}|T + M|\tilde{\psi}\rangle \geqslant \langle\tilde{\psi}|T + M^{\mathrm{ad}}|\tilde{\psi}\rangle \geqslant \tilde{E}^{\mathrm{ad}},$$

where in the last inequality the variational principle has been applied to $T + M^{\mathrm{ad}}$. It follows immediately that any lower bound for the ground state energy of the Hamiltonian

$$-\frac{\omega}{2}\frac{d^2}{dx^2} + \frac{\omega}{2}x^2 - (\tfrac{1}{4}J^2 + 2\alpha^2x^2)^{1/2} + \tfrac{1}{2}(J - \omega) \tag{15}$$

is a lower bound for the ground state energy E of the original Hamiltonian (3). By dropping the kinetic energy in (15) and calculating the minimum of the remaining potential one obtains the lower bound E_{II}. If $4\alpha^2 \leqslant \omega|J|$ one alternatively may approximate the potential in (15) (from below) by a parabola at the origin and thus gets the lower bound E_{IV}.

The lower bound E_{III} may be derived as follows: Consider the two-Boson Hamiltonian

$$\omega b_1^+ b_1 + Jb_2^+ b_2 + \alpha(b_1 + b_1^+)(b_2 + b_2^+), \tag{16}$$

where b_1, b_1^+ and b_2, b_2^+ are the annihilation and creation operators for the first and second Boson, respectively. Expressing the ground state energy of both (3) and (16) by means of the variational principle, one readily sees that the ground state energy E of (3) may be obtained from (16) by restricting the variational principle for (16) to the

tensor product of the Hilbert space of the first Boson and the two-dimensional subspace spanned by the two lowest number states of the second Boson. Thus E is an upper bound for the ground state energy of (16). The latter, however, is nothing but the ground state energy of two linearly coupled harmonic oscillators which is found to be given by E_{III} if $4\alpha^2 \leqslant \omega|J|$; for $4\alpha^2 > \omega|J|$ the Hamiltonian (16) turns out to be unbounded from below and therefore yields only the trivial lower bound $-\infty$ for E.

Finally, the upper bounds E_{V} and E_{VI} represent the variational bounds corresponding to the trial functions

$$e^{\gamma b^+}|0\rangle \otimes |\vartheta+\rangle - e^{-\gamma b^+}|0\rangle \otimes |\vartheta-\rangle,$$

$$e^{\gamma b^+}|0\rangle \otimes (\lambda|\varphi\rangle + (1-\lambda^2)^{1/2}|\chi\rangle)$$

for (3) (with variation parameters γ, respectively γ and λ). Q.E.D.

Figure 2 shows a qualitative plot of the various energy bounds. It seems noteworthy to point out that all relative differences between E_{I}, E_{II}, E_{V}, E_{VI}, and E_{VII} asymptotically tend to zero in the limit $4\alpha^2/\omega|J| \to \infty$.

Finally we mention that lower bounds for E may also be obtained from the fact that the Hamiltonian (3) may be written as the sum of the two exactly solvable Hamiltonians

$$\left.\begin{aligned} &\lambda\omega b^+b + \lambda J c^+c + \alpha(b^+c + bc^+) \\ &(1-\lambda)\omega b^+b + (1-\lambda)Jc^+c + \alpha(b^+c^+ + bc) \end{aligned}\right\} 0 < \lambda < 1,$$

and moreover, by standard methods like Temple's inequality. But we shall not enter into these rather fastidious details which would call for much more computing than is profitable in this oversimplified model.

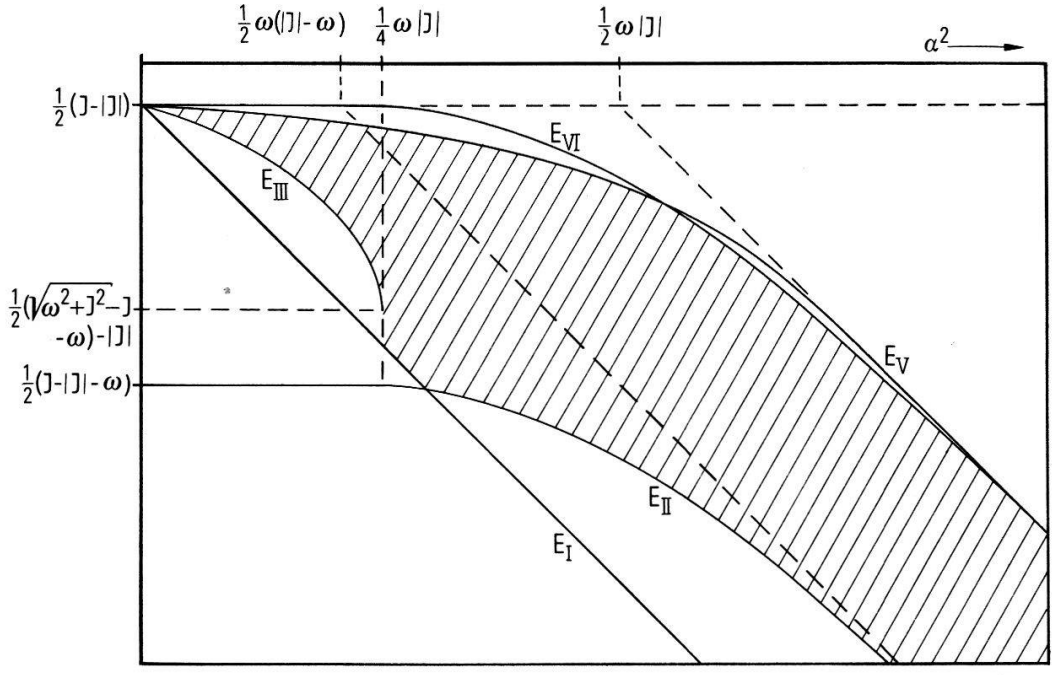

Figure 2
Qualitative plot (for variable α^2 and fixed ω, J) of the various bounds for the ground state energy. The upper and lower line segments enclosing the shaded area represent the respective best upper and lower bounds.

7. Conclusion

A highly simplified model for a magnetic spin system interacting with a vibration mode has been shown to be equivalent to a well-known unsolved one-spin-one-boson Hamiltonian. This was investigated by different methods of approximation in various regions of the parameter space. In the cases $|\alpha| \ll |J|, \omega$ and $|J| \ll \omega$ the eigenvalue problem could be treated by ordinary perturbation theory, yielding merely small energy shifts, with the exception of a resonant phenomenon in the case $|\alpha| \ll |J| = \omega$. More remarkable is the situation of strong coupling, which could only be studied by somewhat dubious and sophisticated methods related to the Born–Oppenheimer approximation. It appears that there then exist two cases for which the behaviour is markedly different: For $\alpha^2 \ll \omega|J|$, the mean phonon occupation number in the ground state is small and the central spin is well localized at the origin. For $\alpha^2 \gg \omega|J|$ in contrast, the mean phonon occupation number in the ground state is extremely large and the system exhibits typical double-well behaviour, i.e. the eigenstates are even or odd linear combinations of coherent states; the central spin is well localised, but away from the origin, and has a non-zero though very small tunnelling frequency to the symmetrical point.

The appearance of coherent states for the eigenfunctions is confirmed by the result that the exact eigenstates behave (in a sense specified earlier) asymptotically like coherent states.

The domain between the above two regions could not be treated. Yet it may be conjectured that the central spin at some stage becomes delocalised, moving simultaneously towards the two points symmetric with respect to the origin, until the tunnelling frequency becomes so small that the central spin may be considered to be displaced from the origin.

It was further shown that the exact ground state has α-independent parity, a non-trivial result in view of the fact that, in the strong coupling case with $\alpha^2 \gg \omega|J|$, the states with odd and even parity are quasi-degenerate with an energy difference decreasing exponentially with α^2/ω.

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